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SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 1/24/03
Art Unit: 1621 Phone Number 30 8 4519 Serial Number: 10/031,486
Mail Box and Bldg/Room Location: CM1 7A07 7E12 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. MEJ

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

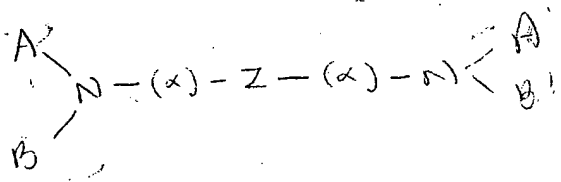
Title of Invention: Quaternary bis ammonium salt precursors and their use as prodrugs

Inventors (please provide full names): Henri Vial et al

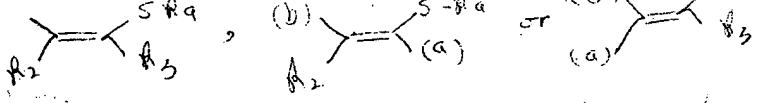
Earliest Priority Filing Date: 7/21/1999

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

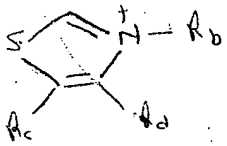


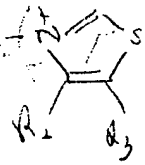
Z is C_6-C_{21} alkylene group optionally interrupted by O, S

α is bond, 

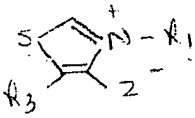
See claim 1 for various definitions.
Also see claims 8, 10, 12, 14, & 15.

Claim 15



R_b is R_1 or T; T is 

R_d is R_2 or P

P is 

R_c is R_3 or H, H is 

****

STAFF USE ONLY

Searcher: AU
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Searcher Location:
Date Searcher Picked Up: 2/3/03
Date Completed: 2/3/03
Searcher Prep & Review Time:
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Type of Search

NA Sequence (#)
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Structure (#) ✓
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Vendors and cost where applicable

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Sequence Systems
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Other (specify)

PTO-1590 (8-01)

BioTech-Chem Library
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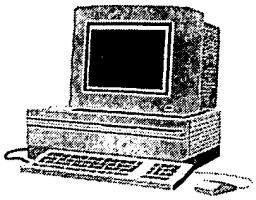
Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact ***the BioTech-Chem searcher*** who conducted the search ***or contact***:

Mary Hale, Supervisor, 308-4258
CM-1 Room 1E01

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* *(Example: 1610)*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

  Types of relevant prior art found:
  - ☐ Foreign Patent(s)
  - ☐ Non-Patent Literature
    (journal articles, conference proceedings, new product announcements etc.)
- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Search results were not useful in determining patentability or understanding the invention.

Other Comments:

Drop off completed forms at the **Circulation Desk CM-1,** or send to Mary Hale, **CM1-1E01 or e-mail mary.hale@uspto.gov.**

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FILE COVERS 1907 - 3 Feb 2003 VOL 138 ISS 6
FILE LAST UPDATED: 2 Feb 2003 (20030202/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d l50 all hitstr

L50 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:63952 HCAPLUS
DN 134:131521
TI Preparation of neutral prodrugs of **bisquaternaryammonium parasiticides**
IN **Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Bourguignon, Jean-Jacques; Vidal, Valerie; Rubi, Eric**
PA Centre National de la Recherche Scientifique (C.N.R.S.), Fr.
SO PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DT Patent
LA French
IC ICM C07C211-09
ICS C07C327-30; C07C323-27; C07C323-59; C07D277-22; C07D277-24; C07D277-30; C07D295-14; A61K031-14; A61K031-145; A61K031-425; A61P033-06; C07D327-06
CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005742	A1	20010125	WO 2000-FR2122	20000721 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	FR 2796642	A1	20010126	FR 1999-9471	19990721 <--
	FR 2796642	B1	20011019		
	EP 1196371	A1	20020417	EP 2000-958598	20000721 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

BR 2000012601 A 20020521 BR 2000-12601 20000721 <--
PRAI FR 1999-9471 A 19990721 <--
WO 2000-FR2122 W 20000721 <--
OS MARPAT 134:131521
AB Title compds., e.g., Z[N(CHO)CR2:CR3SRa]2 [I; Ra = R, SR,COR; R = (un)substituted alkyl, -Ph, heterocyclylmethyl, etc.; R2 = H, alkyl, alkoxycarbonylmethyl; R3 = H, alk(en)yl, etc.; RR3,R2R3 = atoms to complete a ring; Z = (heteroatom- or arylene-interrupted)(satd.) alkylene] were prepd. Thus, 5-(2-hydroxymethyl)-4-methylthiazole was condensed with Br(CH2)12Br to give the bisthiazolium dibromide (drug) which was biscondensed with PrSSO3Na (prepn. given) to give I [Ra = SPr, R2 = Me, R3 = CH2CH2OH, Z = (CH2)12](prodrug). Data for biol. activity of title compds. were given.
ST prodrug **bisquaternaryammonium parasiticide**; **antimalarial bisquaternaryammonium** prodrug
IT **Antimalarials**
Parasiticides
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
IT **321915-72-4P 321915-73-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
IT **321915-74-6P 321915-75-7P 321915-76-8P 321915-77-9P 321915-78-0P 321915-79-1P 321915-80-4P 321915-81-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
IT **321915-50-8P 321915-51-9P 321915-52-0P 321915-53-1P 321915-54-2P 321915-55-3P 321915-56-4P 321915-57-5P 321915-58-6P 321915-59-7P 321915-60-0P 321915-61-1P 321915-62-2P 321915-63-3P 321915-64-4P 321915-65-5P 321915-66-6P 321915-67-7P 321915-68-8P 321915-69-9P 321915-70-2P 321915-71-3P 321915-82-6P 321915-83-7P 321915-84-8P 321915-85-9P 321915-92-8P 321915-93-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
IT 98-88-4, Benzoyl chloride 100-07-2, p-Methoxybenzoyl chloride 100-39-0, Benzyl bromide 106-94-5, Propyl bromide 108-29-2, .gamma.-Valerolactone 109-89-7, Diethylamine, reactions 110-91-8, Morpholine, reactions 137-00-8, 4-Methyl-5-(2-hydroxyethyl)thiazole 141-97-9, Ethyl acetoacetate 629-09-4, 1,6-Diiodohexane 693-95-8, 4-Methylthiazole 1642-81-5, 4-Chloromethylbenzoic acid 3003-84-7, Tetrahydrofurfuryl chloride 3344-70-5, 1,12-Dibromododecane 5259-98-3, 5-Chloro-1-pentanol 7377-26-6, Benzoic acid, 4-chlorocarbonyl, methyl ester 7735-42-4, Hexadecane-1,16-diol
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)

IT 2751-70-4P 6313-36-6P 6363-00-4P 24772-65-4P, 1,12-Diiodododecane
24772-67-6P, 1,16-Diiodohexadecane 51023-75-7P 62642-59-5P
62642-62-0P 77339-73-2P 89585-19-3P 98316-89-3P,
4-Methyl-5-(2-methoxyethyl)thiazole 106261-54-5P 123742-32-5P
321915-86-0P 321915-87-1P 321915-88-2P **321915-89-3P**
321915-90-6P 321915-91-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)

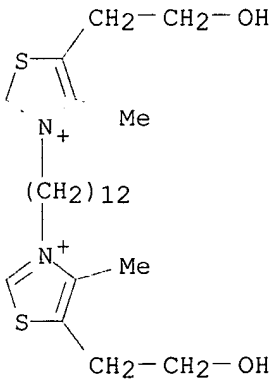
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Hikoichi, H; US 3278537 A 1966
(2) Libman, D; JOURNAL OF THE CHEMICAL SOCIETY 1952, P2305 HCAPLUS
(3) Lopez-Calahorra, F; HETEROCYCLES 1994, V37(3), P1570
(4) Marti; TETRAHEDRON LETT 1993, V34(3), P521 HCAPLUS
(5) Mitchell, R; CHEMICAL ABSTRACTS 1961, V55(12)
(6) Mitchell, R; J PHARMACOL EXPTL THERAP 1961, V131, P334 HCAPLUS
(7) Virbac Sa; FR 2751967 A 1998 HCAPLUS
(8) Zirkle, C; US 3131220 A 1964 HCAPLUS

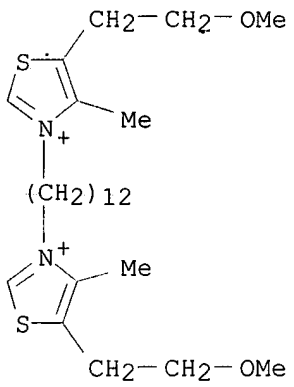
IT **321915-72-4P 321915-73-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)

RN 321915-72-4 HCAPLUS
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-hydroxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)



●2 Br⁻

RN 321915-73-5 HCAPLUS
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)



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IT **321915-74-6P 321915-75-7P 321915-76-8P**
321915-77-9P 321915-78-0P 321915-79-1P
321915-80-4P 321915-81-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
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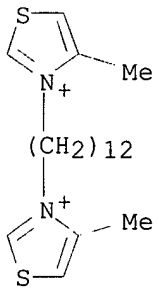
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[4-methyl-, diiodide (9CI) (CA INDEX NAME)



2 I^-

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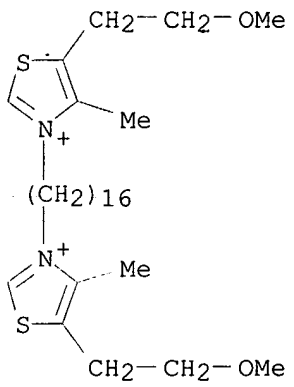

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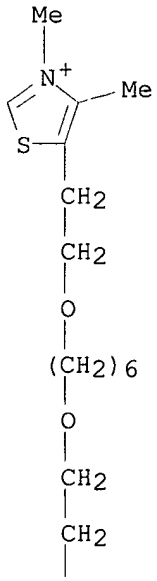
CN Thiazolium, 5,5'-[1,6-hexanediylbis(oxy-2,1-ethanediyl)]bis[3,4-dimethyl-, diiodide (9CI) (CA INDEX NAME)

PAGE 1-A



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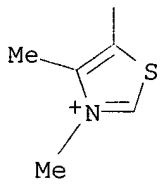

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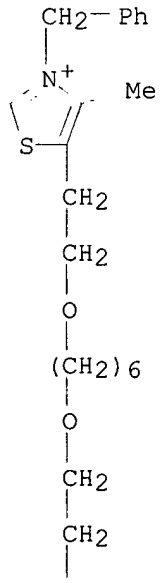
CN Thiazolium, 5,5'-[1,6-hexanediylbis(oxy-2,1-ethanediyl)]bis[4-methyl-3-(phenylmethyl)-, dibromide (9CI) (CA INDEX NAME)

PAGE 1-A



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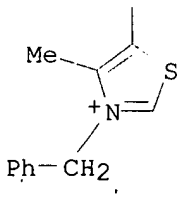

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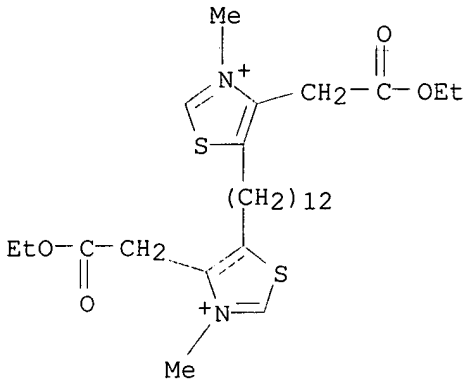

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RN 321915-79-1 HCAPLUS
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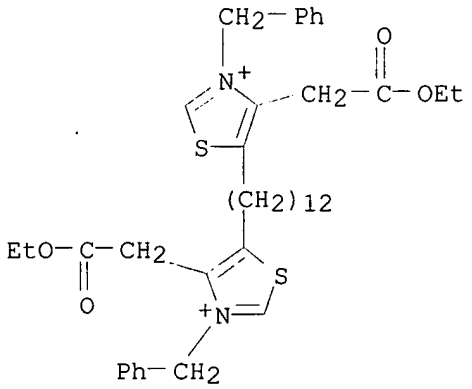

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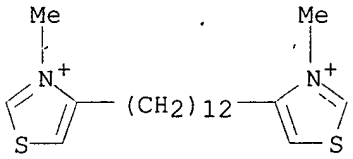
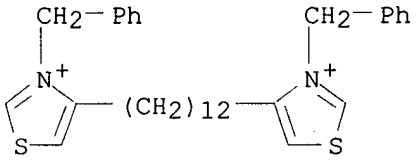


●2 I^-

RN 321915-81-5 HCAPLUS
CN Thiazolium, 4,4'-(1,12-dodecanediyl)bis[3-(phenylmethyl)-, dibromide (9CI) (CA INDEX NAME)



●2 Br^-

IT **321915-50-8P 321915-51-9P 321915-52-0P**
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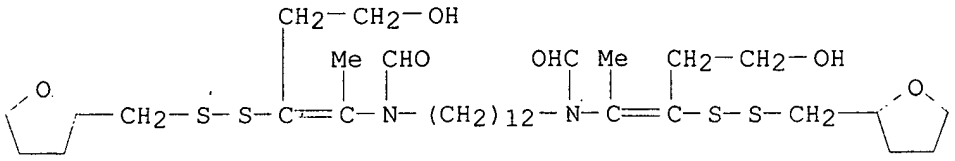
321915-65-5P 321915-66-6P 321915-67-7P
321915-68-8P 321915-69-9P 321915-70-2P
321915-71-3P 321915-82-6P 321915-83-7P
321915-84-8P 321915-85-9P 321915-92-8P
321915-93-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)

RN 321915-50-8 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-[[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]- (9CI) (CA INDEX NAME)



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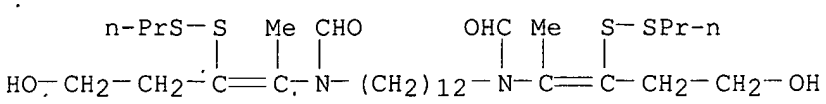

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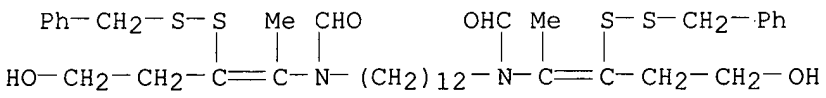
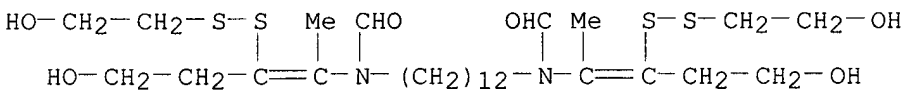
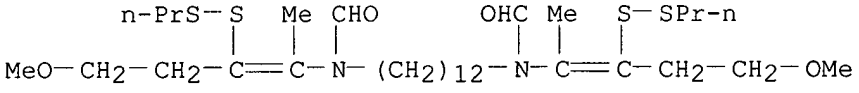


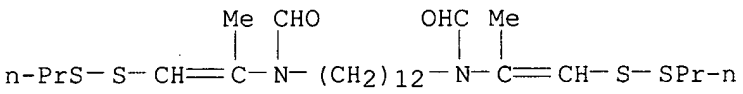
RN 321915-53-1 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-2-[(2-hydroxyethyl)dithio]-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)



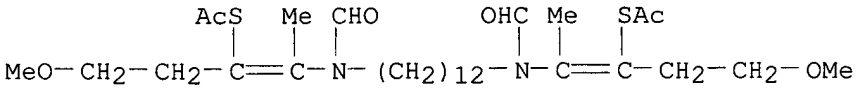
RN 321915-54-2 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-methoxy-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)



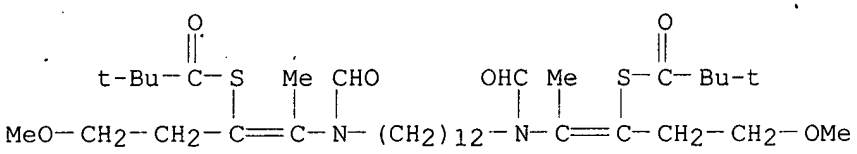
RN 321915-55-3 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[1-methyl-2-(propyldithio)ethenyl]- (9CI) (CA INDEX NAME)



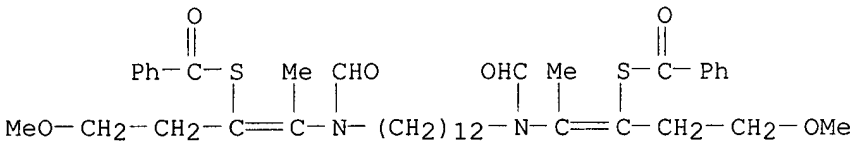
RN 321915-56-4 HCAPLUS
CN Ethanethioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)



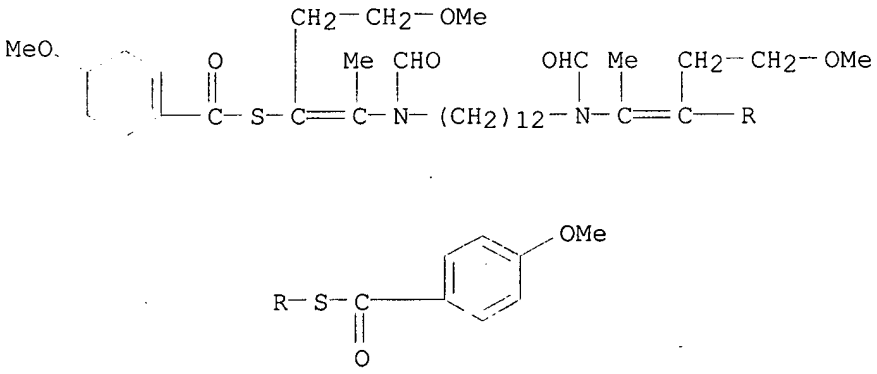
RN 321915-57-5 HCAPLUS
CN Propanethioic acid, 2,2-dimethyl-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)



RN 321915-58-6 HCAPLUS
CN Benzenecarbothioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

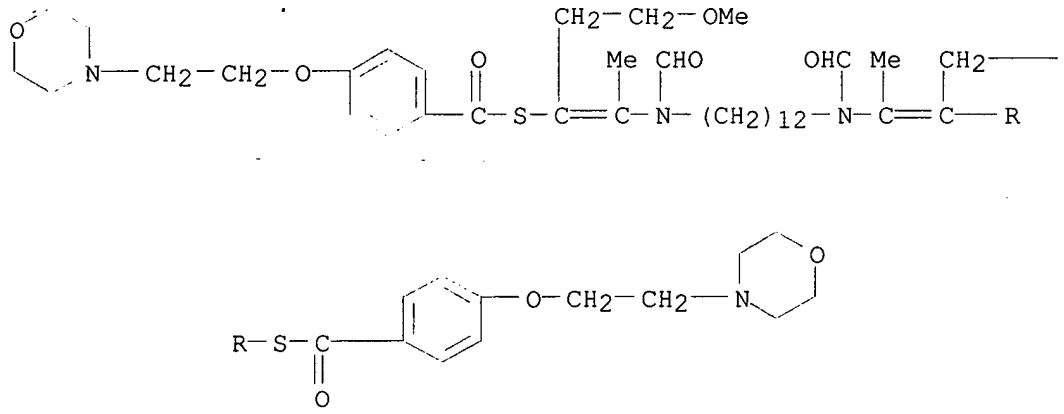


RN 321915-59-7 HCAPLUS
CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)



RN 321915-60-0 HCAPLUS
CN Benzenecarbothioic acid, 4-[2-(4-morpholinyl)ethoxy]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

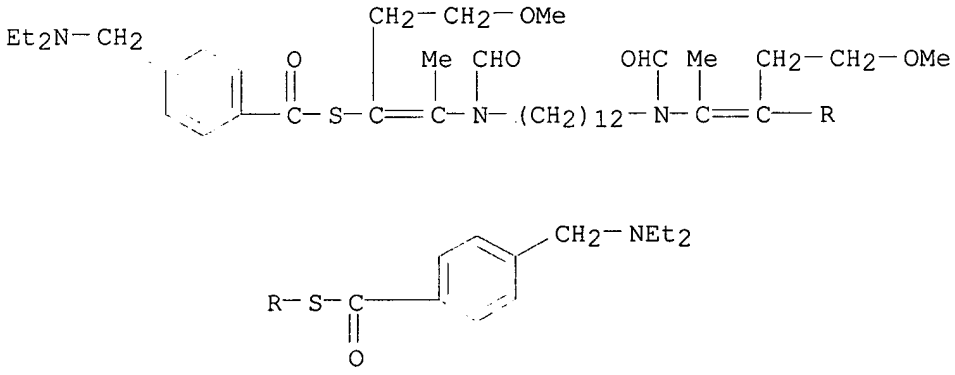
PAGE 1-A



PAGE 1-B

— CH_2 — OMe

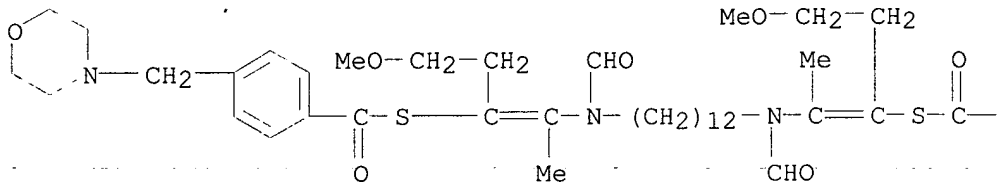
RN 321915-61-1 HCAPLUS
CN Benzenecarbothioic acid, 4-[(diethylamino)methyl]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, dihydrochloride (9CI) (CA INDEX NAME)



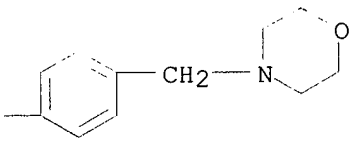
● 2 HCl

RN 321915-62-2 HCAPLUS
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

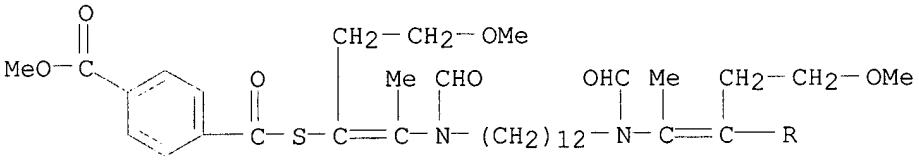
PAGE 1-A

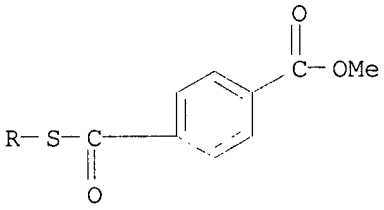


PAGE 1-B

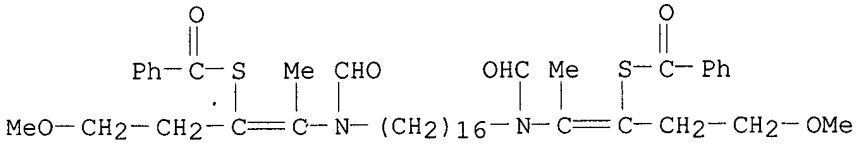


RN 321915-63-3 HCAPLUS
CN Benzoic acid, 4,4'-[5,18-diformyl-3,20-bis(2-methoxyethyl)-4,19-dimethyl-1,22-dioxo-2,21-dithia-5,18-diazadocosa-3,19-diene-1,22-diyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

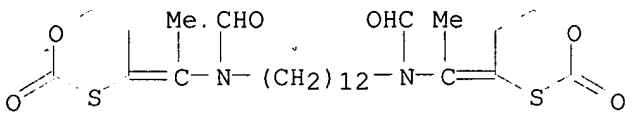




RN 321915-64-4 HCAPLUS
CN Benzenecarbothioic acid, S,S'-[1,16-hexadecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

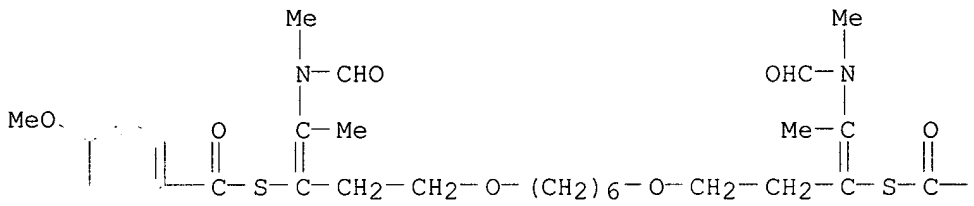


RN 321915-65-5 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[1-(2-oxo-1,3-oxathian-4-ylidene)ethyl]- (9CI) (CA INDEX NAME)



RN 321915-66-6 HCAPLUS
CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,6-hexanediylbis[oxy[1-[1-(formylmethylamino)ethylidene]-3,1-propanediyl]]] ester (9CI) (CA INDEX NAME)

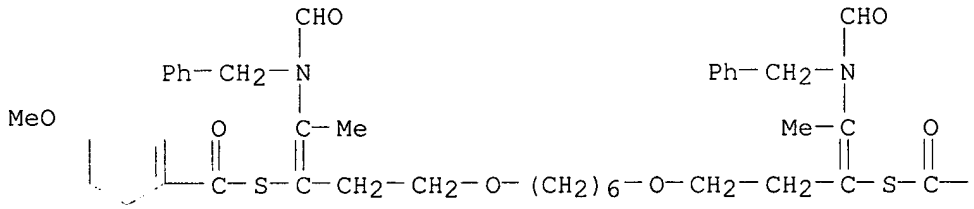
PAGE 1-A



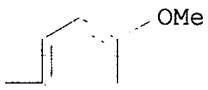
PAGE 1-B

RN 321915-67-7 HCAPLUS
CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,6-hexanediylbis[oxy[1-[1-[formyl(phenylmethyl)amino]ethylidene]-3,1-propanediyl]]] ester (9CI) (CA INDEX NAME)

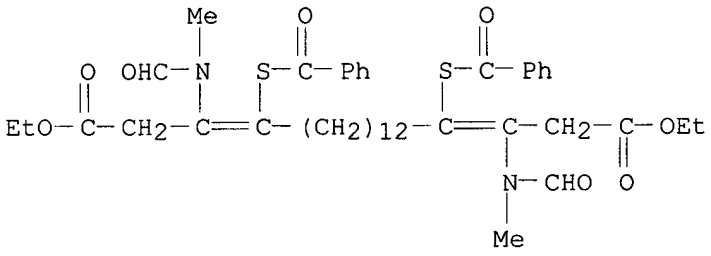
PAGE 1-A



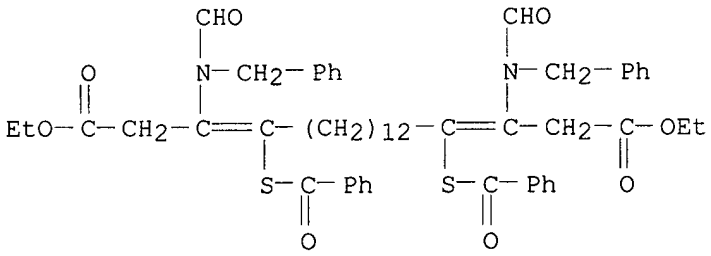
PAGE 1-B



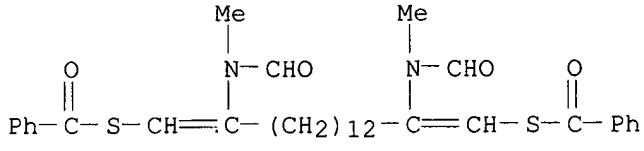
RN 321915-68-8 HCAPLUS
CN 3,17-Eicosadienedioic acid, 4,17-bis(benzoylthio)-3,18-bis(formylmethylamino)-, diethyl ester (9CI) (CA INDEX NAME)



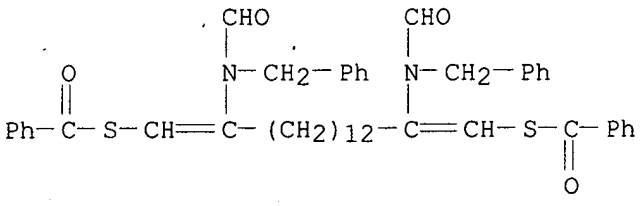
RN 321915-69-9 HCAPLUS
CN 3,17-Eicosadienedioic acid, 4,17-bis(benzoylthio)-3,18-bis[formyl(phenylmethyl)amino]-, diethyl ester (9CI) (CA INDEX NAME)



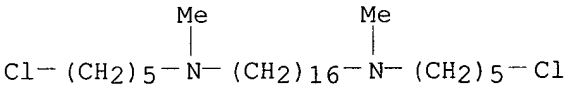
RN 321915-70-2 HCAPLUS
CN Benzenecarbothioic acid, S,S'-[2,15-bis(formylmethylamino)-1,15-hexadecadiene-1,16-diyl] ester (9CI) (CA INDEX NAME)



RN 321915-71-3 HCAPLUS
CN Benzenecarbothioic acid, S,S'-[2,15-bis[formyl(phenylmethyl)amino]-1,15-hexadecadiene-1,16-diyl] ester (9CI) (CA INDEX NAME)

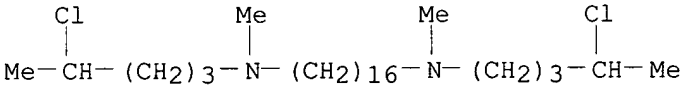


RN 321915-82-6 HCAPLUS
CN 1,16-Hexadecanediamine, N,N'-bis(5-chloropentyl)-N,N'-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 321915-83-7 HCAPLUS
CN 1,16-Hexadecanediamine, N,N'-bis(4-chloropentyl)-N,N'-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



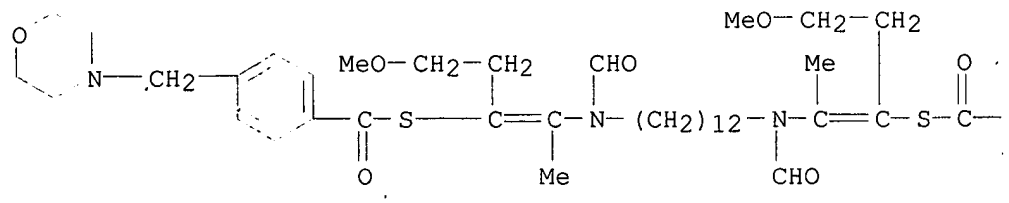
●x HCl

RN 321915-84-8 HCAPLUS
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, ethanedioate (1:2) (9CI) (CA INDEX NAME)

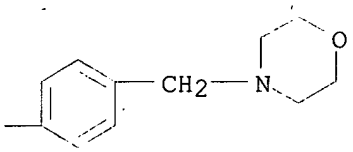
CM 1

CRN 321915-62-2
CMF C50 H74 N4 O8 S2

PAGE 1-A

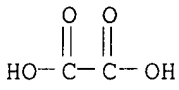


PAGE 1-B



CM 2

CRN 144-62-7
CMF C2 H2 O4

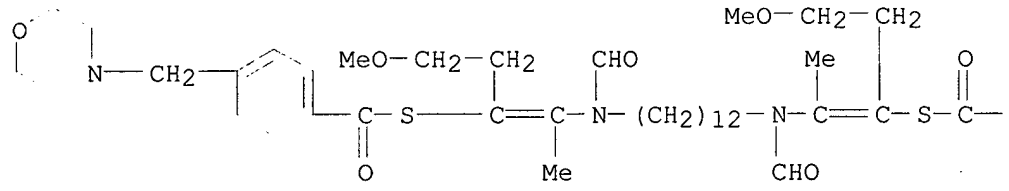


RN 321915-85-9 HCAPLUS
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, (2R,3R)-2,3-dihydroxybutanedioate (1:2) (9CI) (CA INDEX NAME)

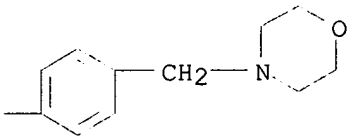
CM 1

CRN 321915-62-2
CMF C50 H74 N4 O8 S2

PAGE 1-A



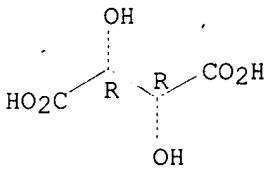
PAGE 1-B



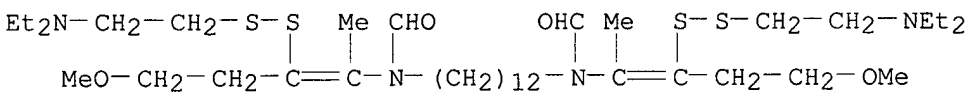
CM 2

CRN 87-69-4
CMF C4 H6 O6

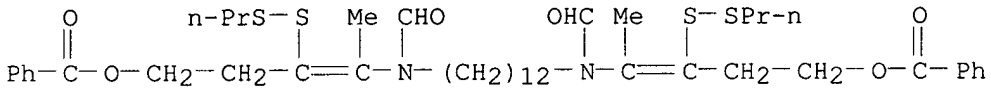
Absolute stereochemistry.



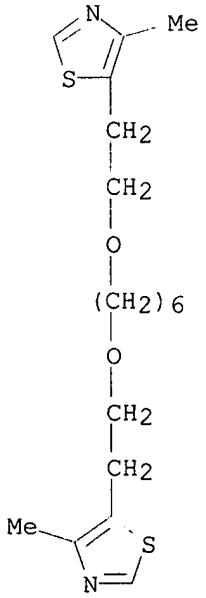
RN 321915-92-8 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[2-[[2-(diethylamino)ethyl]dithio]-4-methoxy-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)



RN 321915-93-9 HCAPLUS
CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-(benzoyloxy)-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)

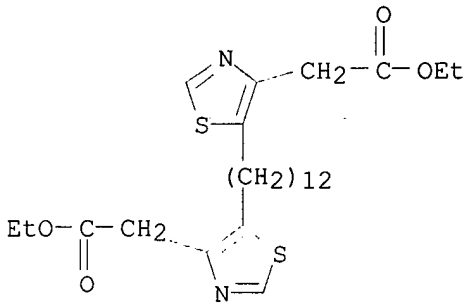


IT **321915-86-0P 321915-89-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of neutral prodrugs of **bisquaternaryammonium parasiticides**)
RN 321915-86-0 HCAPLUS
CN Thiazole, 5,5'-[1,6-hexanediylbis(oxy-2,1-ethanediyl)]bis[4-methyl- (9CI) (CA INDEX NAME)



RN 321915-89-3 HCAPLUS

CN 4-Thiazoleacetic acid, 5,5'-(1,12-dodecanediyl)bis-, diethyl ester (9CI) (CA INDEX NAME)



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L51 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:426419 HCAPLUS
DN 138:32620
TI New drugs against **malaria** with special reference to effectors of **plasmodial** phospholipid metabolism
AU **Vial, Henri J.**; **Vidal-Sailhant, Valerie**; **Ancelin, Marie L.**; Herbute, Serge; Martin, Dominique; Baunaure, F.; **Calas, Michele**
CS UMR 5539 CNRS, Montpellier, 34095, Fr.
SO Multi-Drug Resistance in Emerging and Re-Emerging Diseases, [Joint Symposium on Multiple Drug Resistance and Emerging Diseases], New Delhi, India, Feb. 28-Mar. 4, 1999 (2000), Meeting Date 1999, 175-189. Editor(s): Mahajan, R. C.; Therwath, Amu. Publisher: Indian National Science Academy, New Delhi, India.
CODEN: 69CQYH; ISBN: 81-7319-346-0
DT Conference; General Review
LA English
AB A review. The increasing multidrug resistance of **malarial parasites** to conventional **antimalarial** agents makes very acute the need for novel drugs, since, today, none of them can offer protection against **malaria** in all regions of the world. Drug development efforts generally aim for compds. that work through new, independent mechanisms of action and that are structurally unrelated to existing **antimalarial** agents. From this perspective, thorough biol. and biochem. studies of the **parasite** could lead to the discovery of a specific target that could be used in the design of original compds. capable of exterminating the **parasite** without injuring the host. Phospholipid biosynthesis in **Plasmodium** is of crucial importance considering the high degree of membrane biogenesis. Phospholipid metab. developed by **Plasmodium** during its intraerythrocytic cycle is essential and constitutes a novel pharmacol. target. The most promising interference is the blockade of the choline transporter protein, which provides **Plasmodium** with a precursor for the synthesis of phosphatidylcholine, the major phospholipid of infected erythrocytes. The 1st 2 generations of active lead compds. consisted of **quaternary** ammonium salts and amidine compds. The most prominent characteristics of these new mols. are: potent in vitro **antimalarial** activity against resistant P. **falciparum** strains and isolates, similar in vitro and in vivo activity against P.

vivax, absence of in vitro resistance induction under long-term drug pressure, in vivo activity in various murine species and P. **falciparum**-infected Aotus monkeys even at very high **parasitemia**, lack of recurrence, and absence of genotoxicity. Although tolerance was improved with the 2nd generation of compds., their intestinal absorption remained low. An original strategy has been initiated to design neutral prodrugs which require biotransformation once in the serum compartment (i.e., after passing through the intestinal barrier) to confer **antimalarial** activity. These prodrugs showed the same high in-vitro **antimalarial** activity (nM), tolerance (i.p. LD50 increased by 100-250-fold compared to cationic drugs) and high relative absorption (improved by 10-15-fold compared to cationic drugs). The **antimalarial** activity of these compds. is very satisfactory; all these considerations mean that the approach is now quite realistic. Overall, this pharmacol. approach is novel and should allow the design of candidates for initiating preclin. studies.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 2000:60210 HCAPLUS
DN 132:231503
TI **Antimalarial** Activity of Compounds Interfering with **Plasmodium falciparum** Phospholipid Metabolism: Comparison between Mono- and **Bisquaternary** Ammonium Salts
AU **Calas, Michele**; **Ancelin, Marie L.**; Cordina, Gerard; Portefaix, Philippe; Piquet, Gilles; **Vidal-Sailhan, Valerie**; **Vial, Henri**
CS Laboratoire des Aminoacides Peptides et Proteines, CNRS UMR 5810 Universite de Montpellier II, Montpellier, 34095, Fr.
SO Journal of Medicinal Chemistry (2000), 43(3), 505-516 CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB On the basis of a previous structure-activity relationship study, we identified some essential parameters, e.g. electronegativity and lipophilicity, required for polar head analogs to inhibit **Plasmodium falciparum** phospholipid metab., leading to **parasite** death. To improve the in vitro **antimalarial** activity, 36 cationic choline analogs consisting of mono-, bis-, and **triquaternary** ammonium salts with distinct substituents of increasing lipophilicity were synthesized. For **monoquaternary** ammonium salts, an increase in the lipophilicity around nitrogen was beneficial for **antimalarial** activity: IC50 decreased by 1 order of magnitude from tri-Me to tri-Pr substituents. Irresp. of the polar head substitution (Me, Et, hydroxyethyl, pyrrolidinium), increasing the alkyl chain length from 6 to 12 methylene groups always led to increased activity. The highest activity was obtained for the N,N,N-tripropyl-N-dodecyl substitution of nitrogen (IC50 33 nM). Beyond 12 methylene groups, the **antimalarial** activities of the compds. decreased slightly. The structural requirements for **bisquaternary** ammonium salts in **antimalarial** activity were very similar to those of **monoquaternary** ammonium salts, i.e. polar head steric hindrance and lipophilicity around nitrogen (Me, hydroxyethyl, Et, pyrrolidinium, etc.). In contrast, with **bisquaternary** ammonium salts, increasing the lipophilicity of the alkyl chain between the two nitrogen atoms (from 5 to 21 methylene groups) constantly and dramatically increased the activity. Most of these duplicated mols. had activity around 1 nM, and the most lipophilic compd. synthesized exhibited an IC50 as low as 3 pM (21 methylene groups). Globally, this oriented synthesis produced 28 compds. out of 36 with an IC50 lower than 1 .mu.M, and 9 of them had an IC50 in the nanomolar range, with 1 compd. in the picomolar

range. This indicates that developing a pharmacol. model for **antimalarial** compds. through choline analogs is a promising strategy.
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 1998:105729 HCAPLUS
DN 128:238968
TI **Antimalarial** activity of 77 phospholipid polar head analogs: close correlation between inhibition of phospholipid metabolism and in vitro **Plasmodium falciparum** growth
AU **Ancelin, Marie L.**; **Calas, Michele**; Bompart, Jacques; Cordina, Gerard; Martin, Dominique; Bari, Mohammed Ben; Jei, Taib; Druilhe, Pierre; **Vial, Henri J.**
CS CNRS UMR 5539, Department of Biologie-Sante, Montpellier, 34095, Fr.
SO Blood (1998), 91(4), 1426-1437
CODEN: BLOOAW; ISSN: 0006-4971
PB W. B. Saunders Co.
DT Journal
LA English
AB Seventy-seven potential analogs of phospholipid polar heads, choline and ethanolamine, were evaluated in vitro as inhibitors of **Plasmodium falciparum** growth. Their IC50 ranged from 10-3 to 10-7 mol/L. Ten compds. showed similar **antimalarial** activity when tested against three different **parasite** strains (2 chloroquine-sensitive strains and 1 chloroquine-resistant strain). Compds. showing marked **antimalarial** activity were assayed for their effects on phospholipid metab. The most active compds. (IC50 of 1 to 0.03 .mu.mol/L) were inhibitors of de novo phosphatidylcholine (PC) biosynthesis from choline. For a series of 50 compds., there was a close correlation between impairment of phospholipid biosynthesis and inhibition of in vitro **malaria parasite** growth. High choline concns. caused a marked specific shift in the curves for PC biosynthesis inhibition. Concns. inhibiting 50% PC metab. from choline were in close agreement with the Ki of these compds. for the choline transporter in **Plasmodium** knowlesi-infected erythrocytes. By contrast, measurement of the effects of 12 of these compds. on rapidly dividing lymphoblastoid cells showed a total absence of correlation between **parasite** growth inhibition and human lymphoblastoid cell growth inhibition. Specific **antimalarial** effects of choline or ethanolamine analogs are thus likely mediated by their alteration of phospholipid metab. This indicates that de novo PC biosynthesis from choline is a very realistic target for new **malaria** chemotherapy, even against pharmacoresistant strains.

L51 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 1998:98316 HCAPLUS
DN 128:127745
TI Preparation of .alpha.,.omega.-bis(**quaternary** ammonium)alkane salt **antimalarial** and **antibabesiasis** agents
IN **Vial, Henri**; **Calas, Michele**; **Ancelin, Marie-Laure**; Giral, Louis
PA Virbac S.A., Fr.; Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Giral, Louis
SO PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9804252	A1	19980205	WO 1997-FR1336	19970717

W: BR, CA, CN, JP, KR, US
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

	FR 2751967	A1	19980206	FR 1996-9678	19960731
	FR 2751967	B1	19981009		
	EP 917465	A1	19990526	EP 1997-934589	19970717
	EP 917465	B1	20021120		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	BR 9710629	A	19990817	BR 1997-10629	19970717
	CN 1232388	A	19991020	CN 1997-197753	19970717
	JP 2000515877	T2	20001128	JP 1998-508541	19970717
	AT 227984	E	20021215	AT 1997-934589	19970717
	US 6096788	A	20000801	US 1999-240627	19990201
	KR 2000029690	A	20000525	KR 1999-700769	19990929
PRAI	FR 1996-9678	A	19960731		
	WO 1997-FR1336	W	19970717		

OS MARPAT 128:127745

AB The title compds. R1(R2)(R3)N+XN+(R3)(R2)R1 [I; R1 = C1-20 hydrocarbyl; R2, R3 = (un)substituted C1-20 hydrocarbyl; X = (un)substituted C12-26 dihydrocarbyl; counterion definitions not presented], having **antimalarial** and (veterinarian) **antibabesiasis** (e.g., anti-piroplasmosis) activities, are prepd. and a I-contg. formulation claimed. Thus, 1,21-dibromoheneicosane was reacted with MeNEt2, producing N,N'-dimethyl-N,N,N',N'-tetraethyl-1,21-heneicosanediammonium dibromide (m.p. 205), which demonstrated an in-vitro IC50 assay of 0.000003 .mu.M against Babesia bovis and Babesia canis and a therapeutic index of 12.

L51 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 1997:638456 HCAPLUS
DN 127:287699
TI **Antimalarial** Activity of Molecules Interfering with **Plasmodium falciparum** Phospholipid Metabolism. Structure-Activity Relationship Analysis
AU **Calas, Michele**; Cordina, Gerard; Bompart, Jacques; Bari, Mohamed Ben; Jei, Taieb; **Ancelin, Marie L.**; **Vial, Henri**
CS Laboratoire des Aminoacides Peptides et Proteines, ESA CNRS 5075, Montpellier, Fr.
SO Journal of Medicinal Chemistry (1997), 40(22), 3557-3566
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English

AB A series of 80 compds., primary, secondary, and tertiary amines and **quaternary** ammonium and bisammonium salts, most of them synthesized as potential choline or ethanolamine analogs, were tested against the in vitro growth of **Plasmodium falciparum**, the human **malaria parasite**. They were active over the 10-3-10-8 M concn. range. A structure-activity relationship study was carried out using autocorrelation vectors as structural descriptors, and multidimensional anal. Principal component anal., ascending hierarchical classification, and stepwise discriminant anal. showed that both the size and shape of the mol. were essential for **antimalarial** potency, making the lipophilicity and electronegativity distribution in the mol. space essential. Using the autocorrelogram describing the mol. shape and the electronegativity distribution on the mol. graph, 98% of the mols. were correctly classified either as poorly active or active with only three explanatory variables. The most active compds. were **quaternary** ammoniums salts whose nitrogen atom had only one long lipophilic chain of 11 or 12 methylene groups or the bisammoniums whose polar heads were linked by linear alkyl chains of 10 to 12 carbon atoms. The hydroxyethyl group of choline was not very beneficial, whereas the charge and substitutions of nitrogen (aimed at increasing lipophilicity) were essential for optimal interactions. A crude topog. model of the

ligand (choline) binding site was thus drawn up.

L51 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS
AN 1986:403415 HCAPLUS
DN 105:3415
TI **Quaternary** ammonium compounds efficiently inhibit **Plasmodium falciparum** growth in vitro by impairment of choline transport
AU **Ancelin, Marie L.; Vial, Henri J.**
CS Cent. Natl. Rech. Sci., Inst. Natl. Sante Rech. Med., Montpellier, 34100, Fr.
SO Antimicrobial Agents and Chemotherapy (1986), 29(5), 814-20
CODEN: AMACCQ; ISSN: 0066-4804
DT Journal
LA English
AB Hemicholinium 3, decamethonium, and decyltrimethylammonium previously were demonstrated to be efficient inhibitors of P. **falciparum**, with 50% inhibitory concns. of 4 .times. 10-6, 10-6, and 7 .times. 10-7M, resp. Lengthening of the alkyl chain of decyltrimethylammonium by successive addns. of 2 C atoms up to hexadecyltrimethylammonium resulted in a very low 50% inhibitory concn. of 5 .times. 10-7 M for dodecyltrimethylammonium. Hemicholinium 3 and decamethonium exerted their **antiplasmodial** activity regardless of the developmental stage of the **parasite**, whereas decyltrimethylammonium was particularly lethal for the mature forms. After infected erythrocytes with radioactive choline were supplied, the detn. of the water-sol. choline-contg. compds. as well as the assay of choline kinase activity showed that the specific inhibition of phosphatidylcholine biosynthesis is related to the impairment of choline entry into erythrocytes. Thus, the impairment of the transport of choline, a natural polar head group of phospholipids, appears to be lethal for P. **falciparum** in vitro and could be a reasonable approach for a new **malaria** chemotherapy.

=> d his

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E WO2000-FR2122/AP,PRN
L2 1 S E3,E4
L3 1 S L1,L2
SEL RN

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L5 4 S L4 AND CLH
L6 2 S L5 NOT C6/ES
L7 3 S L5 NOT C12H17NO2
L8 1 S L7 NOT L6
L9 70 S L4 NOT L5
L10 25 S L9 AND 1 12 DODECANE?
L11 10 S L10 AND C6/ES
L12 8 S L11 NOT NCSC2/ES
L13 6 S L12 AND 1/NC
L14 4 S L11 NOT L13
L15 2 S L14 NOT BR/ELS
L16 15 S L10 NOT L11-L15
L17 9 S L16 NOT NCSC2/ES
L18 45 S L9 NOT L10-L17

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L19          38 S L18 NOT NCSC2/ES
L20          17 S L19 AND N/ELS
L21           8 S L20 AND S/ELS
L22           9 S L20 NOT L21
L23          28 S L18 NOT L20-L22
L24           7 S L23 AND NCSC2/ES
L25          28 S L7,L8,L13,L15,L17,L21
L26           4 S L24 AND NR>=2
L27          39 S L4 NOT L24-L26
L28           8 S L27 AND NCSC2/ES
L29          31 S L27 NOT L28
L30          15 S L24,L28

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L35           1 S L34 AND L1-L3
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L36          85 S E3-E8
                E CALAS M/AU
L37          31 S E3-E5,E8
                E ANCELIN M/AU
L38          41 S E3,E4,E6,E7
                E BOURGUIGNON J/AU
L39         204 S E3,E5,E10,E12
                E VIDAL V/AU
L40          34 S E3-E9,E14,E15
                E RUBI E/AU
L41          13 S E3,E5
L42           1 S L35 AND L36-L41
L43          20 S L36-L41 AND (QUAT OR ?QUATERN?)
                E VIDAL SAILHANT V/AU
L44           1 S E4
L45           1 S E2
                E SAILHAN/AU
L46           3 S E4,E5
L47          20 S L36-L41,L44-L46 AND (QUAT OR ?QUATER?)
L48          20 S L43,L47
L49           7 S L48 AND (?MALAR? OR ?PLASMOD? OR ?FALCIPAR? OR ?PARASIT? OR ?
L50           1 S L35 AND L36-L49
L51           6 S L49 NOT L50
                SEL RN

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L52         255 S E1-E255

     FILE 'HCAPLUS' ENTERED AT 16:57:54 ON 03 FEB 2003
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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:20:32 ON 05 FEB 2003

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:20:43 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5
DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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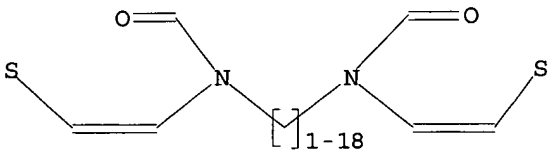

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

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FULL SCREEN SEARCH COMPLETED -      45 TO ITERATE

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SEARCH TIME: 00.00.01

L3            19 SEA SSS FUL L1

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RN   321915-54-2  REGISTRY
CN   Formamide, N,N'-1,12-dodecanediylbis[N-[4-methoxy-1-methyl-2-
     (propyldithio)-1-butenyl]- (9CI)  (CA INDEX NAME)
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MF   C32 H60 N2 O4 S4
SR   CA
LC   STN Files:   CA, CAPLUS
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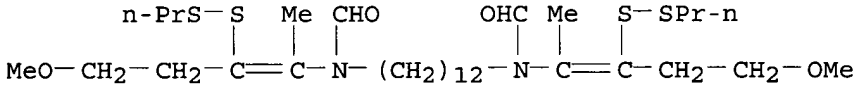

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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               1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3   ANSWER 16 OF 19  REGISTRY  COPYRIGHT 2003 ACS
RN   321915-53-1  REGISTRY
CN   Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-2-[(2-
     hydroxyethyl)dithio]-1-methyl-1-butenyl]- (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C28 H52 N2 O6 S4
SR   CA
LC   STN Files:   CA, CAPLUS
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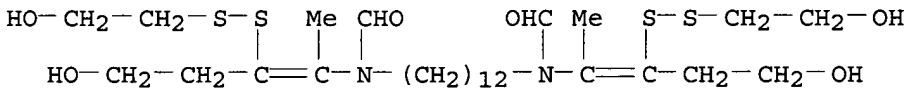

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L3   ANSWER 17 OF 19  REGISTRY  COPYRIGHT 2003 ACS
RN   321915-52-0  REGISTRY
CN   Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-
     [(phenylmethyl)dithio]-1-butenyl]- (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C38 H56 N2 O4 S4
SR   CA
LC   STN Files:   CA, CAPLUS
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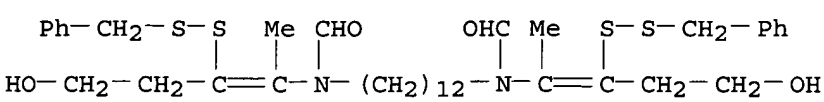

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L3 ANSWER 18 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-51-9 REGISTRY
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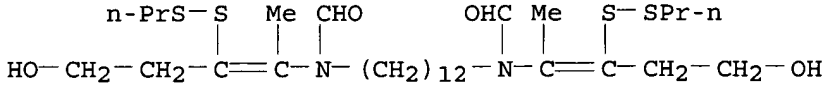
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 19 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-50-8 REGISTRY
CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-[[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]- (9CI) (CA INDEX NAME)
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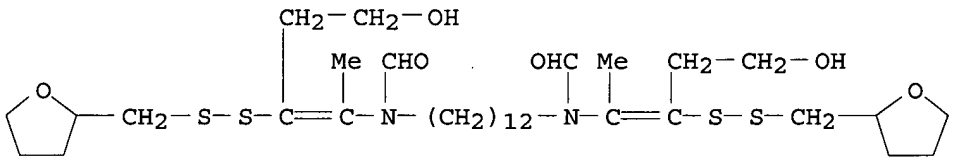
SR CA
LC STN Files: CA, CAPLUS



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L3 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-93-9 REGISTRY
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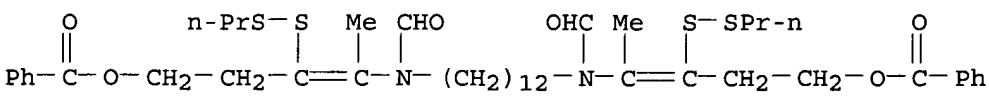
SR CA
LC STN Files: CA, CAPLUS



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L3 ANSWER 2 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-92-8 REGISTRY
CN Formamide, N,N'-1,12-dodecanediylbis[N-[2-[[2-(diethylamino)ethyl]dithio]-4-methoxy-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
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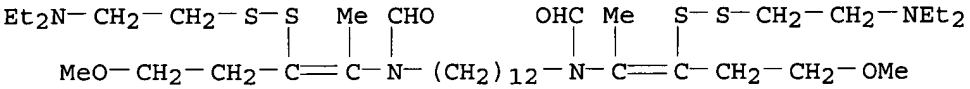
SR CA
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 3 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-85-9 REGISTRY
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, (2R,3R)-2,3-dihydroxybutanedioate (1:2) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C50 H74 N4 O8 S2 . 2 C4 H6 O6
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 321915-62-2
CMF C50 H74 N4 O8 S2

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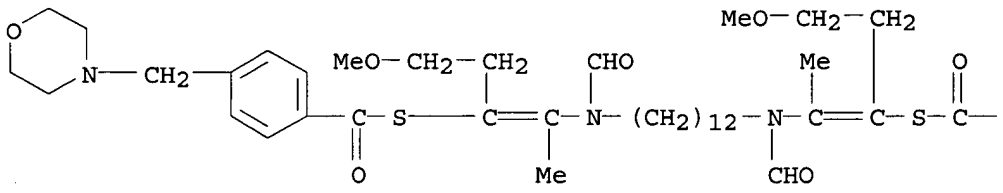

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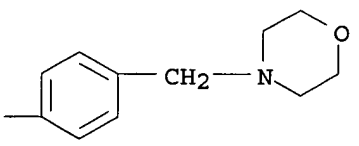

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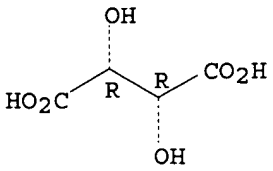
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 4 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-84-8 REGISTRY
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, ethanedioate (1:2) (9CI) (CA INDEX NAME)
MF C50 H74 N4 O8 S2 . 2 C2 H2 O4
SR CA
LC STN Files: CA, CAPLUS

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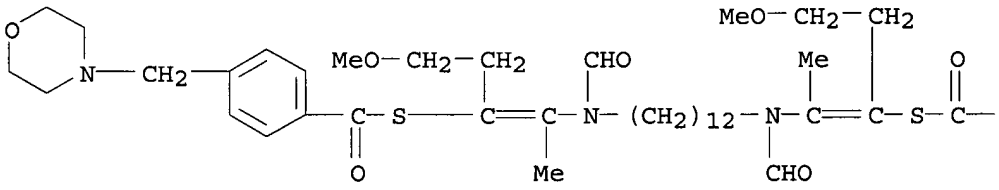
CRN 321915-62-2
CMF C50 H74 N4 O8 S2

PAGE 1-A



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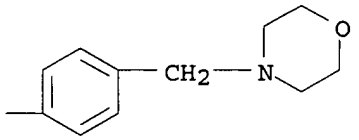
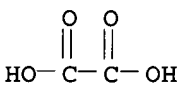


CM 2

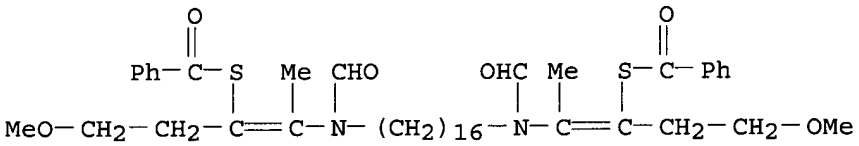
CRN 144-62-7
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 5 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-64-4 REGISTRY
CN Benzenecarbothioic acid, S,S'-[1,16-hexadecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C44 H64 N2 O6 S2
SR CA

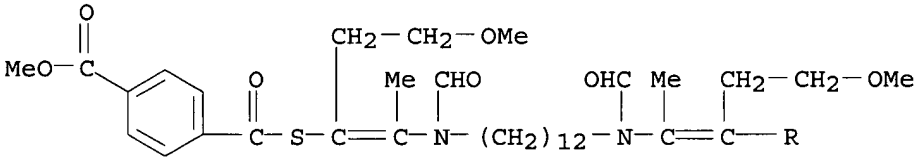
LC STN Files: CA, CAPLUS

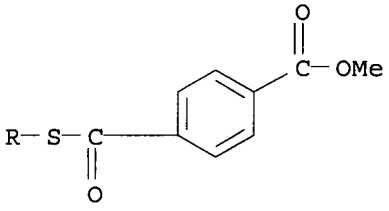


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 6 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-63-3 REGISTRY
CN Benzoic acid, 4,4'-[5,18-diformyl-3,20-bis(2-methoxyethyl)-4,19-dimethyl-1,22-dioxo-2,21-dithia-5,18-diazadocosa-3,19-diene-1,22-diyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)
MF C44 H60 N2 O10 S2
SR CA
LC STN Files: CA, CAPLUS

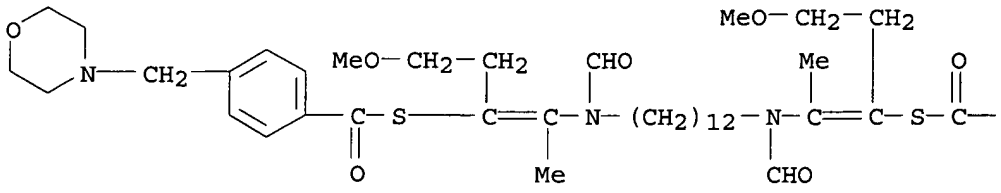




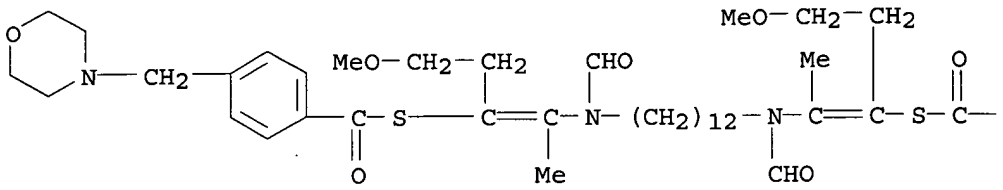
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

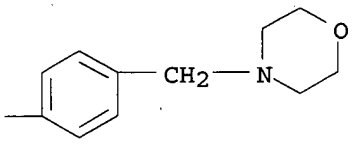
L3 ANSWER 7 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-62-2 REGISTRY
CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C50 H74 N4 O8 S2
CI COM
SR CA
LC STN Files: CA, CAPLUS



PAGE 1-A



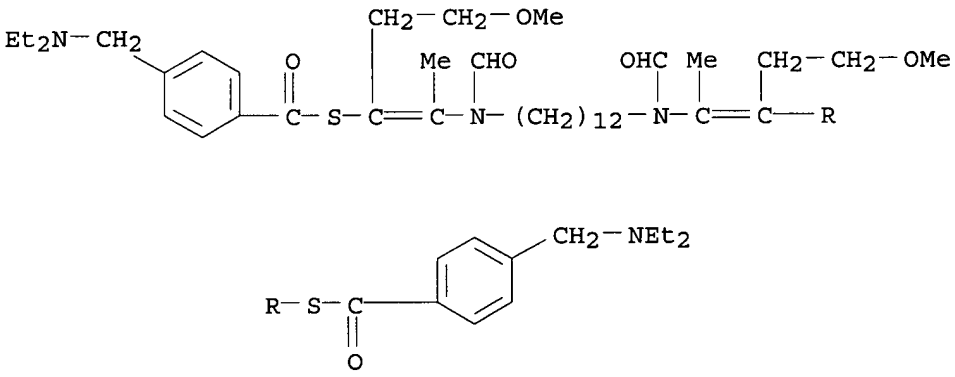
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 8 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-61-1 REGISTRY
CN Benzenecarbothioic acid, 4-[(diethylamino)methyl]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, dihydrochloride (9CI) (CA INDEX NAME)
MF C50 H78 N4 O6 S2 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS

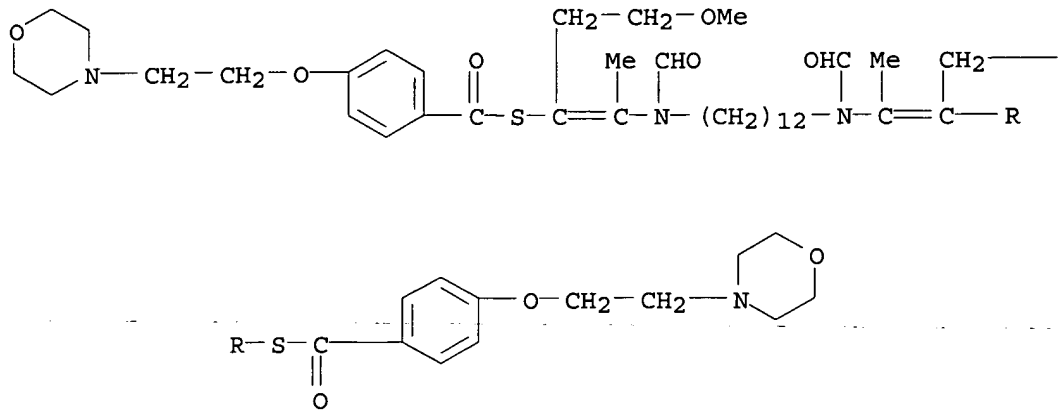


●2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 9 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-60-0 REGISTRY
CN Benzenecarbothioic acid, 4-[2-(4-morpholinyl)ethoxy]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C52 H78 N4 O10 S2
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



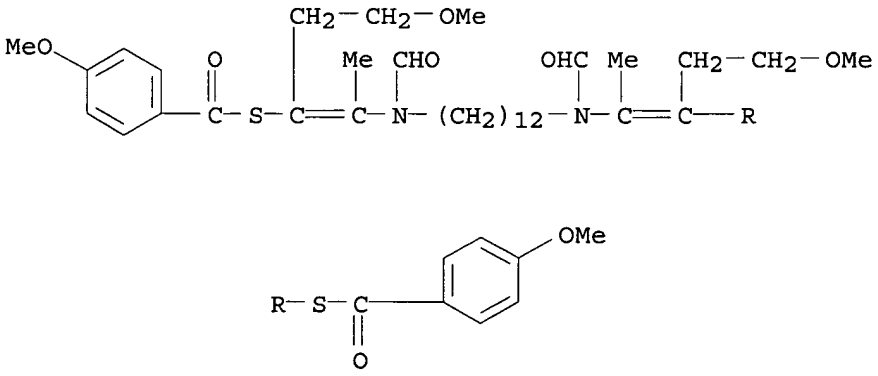
PAGE 1-B

— CH_2 — OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

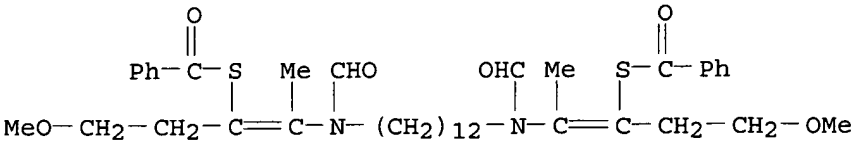
L3 ANSWER 10 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-59-7 REGISTRY
CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C42 H60 N2 O8 S2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

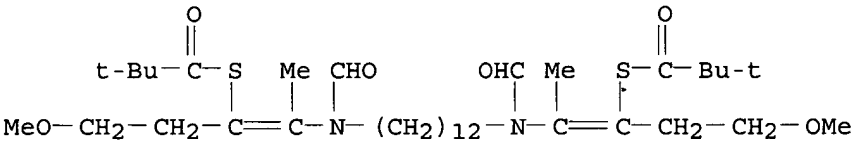
L3 ANSWER 11 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-58-6 REGISTRY
CN Benzenecarbothioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C40 H56 N2 O6 S2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

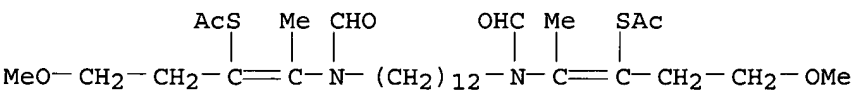
L3 ANSWER 12 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-57-5 REGISTRY
CN Propanethioic acid, 2,2-dimethyl-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C36 H64 N2 O6 S2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

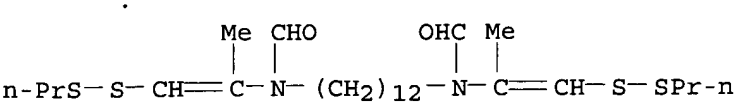
L3 ANSWER 13 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-56-4 REGISTRY
CN Ethanethioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
MF C30 H52 N2 O6 S2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 14 OF 19 REGISTRY COPYRIGHT 2003 ACS
RN 321915-55-3 REGISTRY
CN Formamide, N,N'-1,12-dodecanediylbis[N-[1-methyl-2-(propyldithio)ethenyl]-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H48 N2 O2 S4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	180.47	180.68

FILE 'CAPLUS' ENTERED AT 16:21:51 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 5 Feb 2003 VOL 138 ISS 6
FILE LAST UPDATED: 4 Feb 2003 (20030204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
AN 2001:63952 CAPLUS
DN 134:131521
TI Preparation of neutral prodrugs of bisquaternaryammonium parasiticides
IN Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Bourguignon, Jean-Jacques; Vidal, Valerie; Rubi, Eric
PA Centre National de la Recherche Scientifique (C.N.R.S.), Fr.
SO PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001005742	A1	20010125	WO 2000-FR2122	20000721

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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     FR 2796642         A1   20010126       FR 1999-9471     19990721
     FR 2796642         B1   20011019
     EP 1196371         A1   20020417       EP 2000-958598   20000721
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     BR 2000012601      A    20020521       BR 2000-12601    20000721
PRAI FR 1999-9471       A    19990721
     WO 2000-FR2122     W    20000721
OS   MARPAT 134:131521
RE.CNT  8      THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> file caold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     1.43     182.11

FILE 'CAOLD' ENTERED AT 16:22:26 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=> s l3
L5            0 L3
```

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:27:26 ON 05 FEB 2003

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:27:36 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5
DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

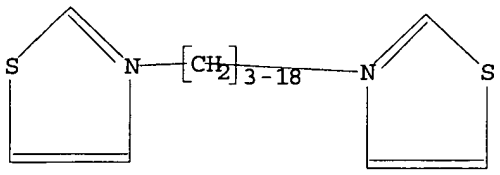
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 486.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:27:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 143 TO ITERATE

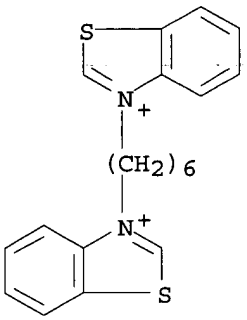
100.0% PROCESSED 143 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2143 TO 3577
PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> d l2 5

L2 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 47358-00-9 REGISTRY
CN Benzothiazolium, 3,3'-(1,6-hexanediyl)bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 N2 S2
CI COM



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.88	3.09

FILE 'STNGUIDE' ENTERED AT 16:29:10 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 31, 2003 (20030131/UP).

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	3.15

FILE 'REGISTRY' ENTERED AT 16:29:50 ON 05 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5
DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

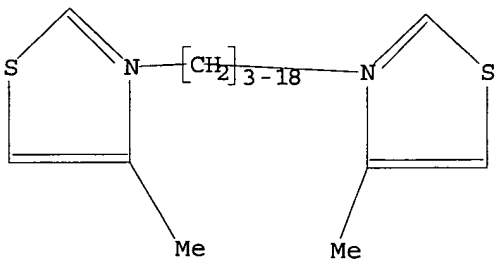
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 486.str

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3
SAMPLE SEARCH INITIATED 16:30:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

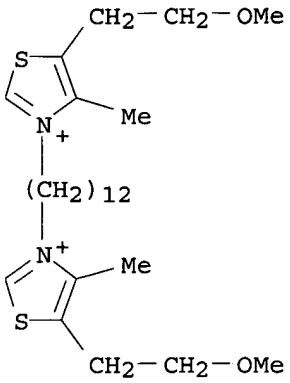
100.0% PROCESSED 9 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9 TO 360
PROJECTED ANSWERS: 1 TO 80

L4 1 SEA SSS SAM L3

=> d

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN 321915-73-5 REGISTRY
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C26 H46 N2 O2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



2 Br^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

```
=> s l3 ful
FULL SEARCH INITIATED 16:30:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    266 TO ITERATE

100.0% PROCESSED     266 ITERATIONS                          22 ANSWERS
SEARCH TIME: 00.00.01

L5            22 SEA SSS FUL L3

=> d l5 1-22

L5   ANSWER 1 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   477526-11-7  REGISTRY
CN   INDEX NAME NOT YET ASSIGNED
MF   C26 H32 N4 S2 . 2 Br
SR   Chemical Library
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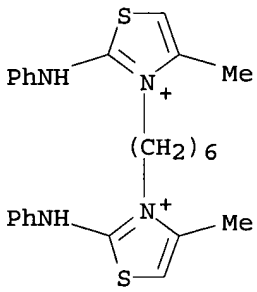

2 Br^-

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L5   ANSWER 2 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   321915-75-7  REGISTRY
CN   Thiazolium, 3,3'-(1,16-hexadecanediyl)bis[5-(2-methoxyethyl)-4-methyl-,
     diiodide (9CI)  (CA INDEX NAME)
MF   C30 H54 N2 O2 S2 . 2 I
SR   CA
LC   STN Files:   CA, CAPLUS
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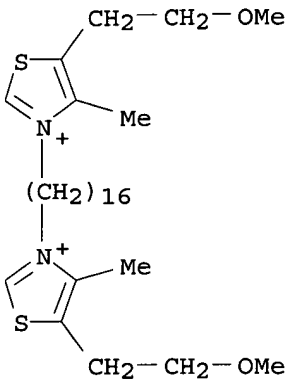
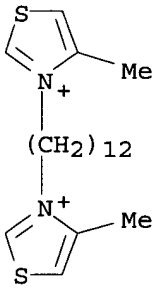


2 I^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

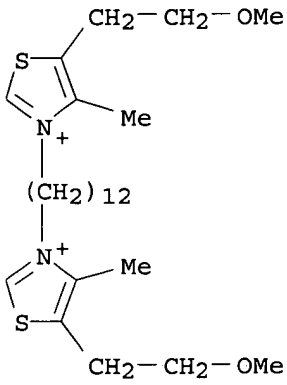
L5 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 321915-74-6 REGISTRY
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[4-methyl-, diiodide (9CI) (CA INDEX NAME)
MF C20 H34 N2 S2 . 2 I
SR CA
LC STN Files: CA, CAPLUS



2 I^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 321915-73-5 REGISTRY
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C26 H46 N2 O2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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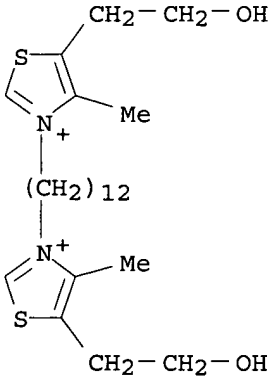
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 321915-72-4 REGISTRY
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-hydroxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C24 H42 N2 O2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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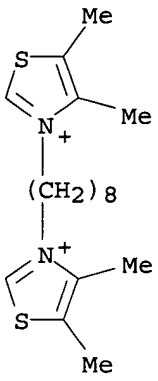
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-88-5 REGISTRY
CN Thiazolium, 3,3'-(1,8-octanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C18 H30 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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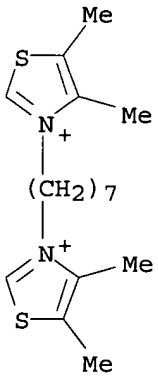
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-87-4 REGISTRY
CN Thiazolium, 3,3'-(1,7-heptanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C17 H28 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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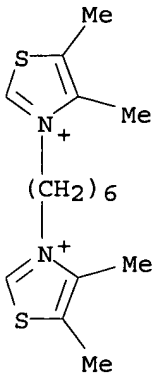
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-86-3 REGISTRY
CN Thiazolium, 3,3'-(1,6-hexanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C16 H26 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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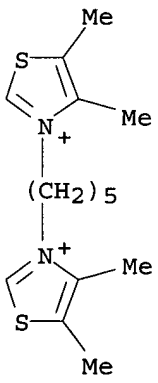
3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-85-2 REGISTRY
CN Thiazolium, 3,3'-(1,5-pentanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C15 H24 N2 S2 . 2 Br
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



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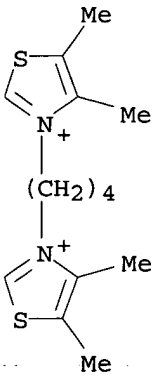
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-84-1 REGISTRY
CN Thiazolium, 3,3'-(1,4-butanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C14 H22 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



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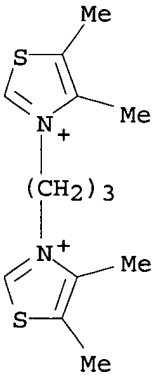
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

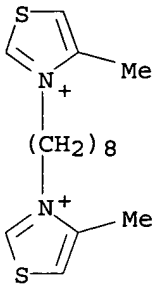
L5 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 146891-83-0 REGISTRY
CN Thiazolium, 3,3'-(1,3-propanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
MF C13 H20 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



2 Br^-

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

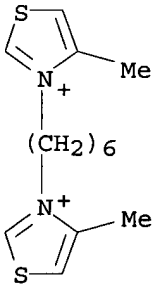
L5 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 105420-27-7 REGISTRY
CN Thiazolium, 3,3'-(1,8-octanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C16 H26 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



2 Br^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

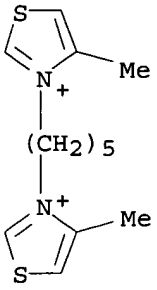
L5 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 105420-26-6 REGISTRY
CN Thiazolium, 3,3'-(1,6-hexanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C14 H22 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS



2 Br^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

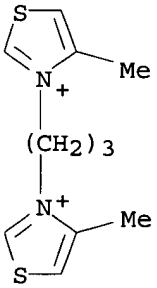
L5 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 105420-25-5 REGISTRY
CN Thiazolium, 3,3'-(1,5-pentanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C13 H20 N2 S2 . 2 Br
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



●2 Br⁻

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

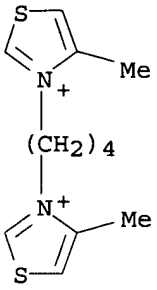
L5 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 105420-24-4 REGISTRY
CN Thiazolium, 3,3'-(1,3-propanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C11 H16 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS, CASREACT



2 Br⁻

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

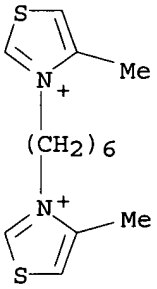
L5 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 97745-74-9 REGISTRY
CN Thiazolium, 3,3'-(1,4-butanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)
MF C12 H18 N2 S2 . 2 Br
SR CA
LC STN Files: CA, CAPLUS, CASREACT



●2 Br^-

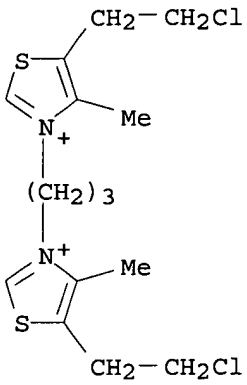
3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 87051-17-0 REGISTRY
CN Thiazolium, 3,3'-(1,6-hexanediyl)bis[4-methyl-, dichloride (9CI) (CA INDEX NAME)
MF C14 H22 N2 S2 . 2 Cl



●2 Cl^-

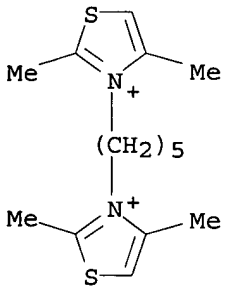
L5 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 76800-93-6 REGISTRY
CN Thiazolium, 3,3'-(1,3-propanediyl)bis[5-(2-chloroethyl)-4-methyl-, diiodide (9CI) (CA INDEX NAME)
MF C15 H22 Cl2 N2 S2 . 2 I
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



2 I^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 54642-19-2 REGISTRY
CN Thiazolium, 3,3'-(1,5-pentanediyl)bis[2,4-dimethyl-, dibromide (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3,3'-Pentamethylenebis(2,4-dimethylthiazolium bromide)
MF C15 H24 N2 S2 . 2 Br
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



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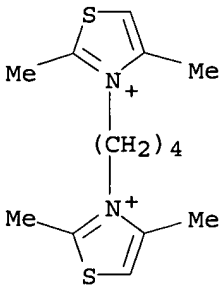
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 54642-18-1 REGISTRY
CN Thiazolium, 3,3'-(1,4-butanediyl)bis[2,4-dimethyl-, diiodide (9CI) (CA INDEX NAME)
MF C14 H22 N2 S2 . 2 I
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



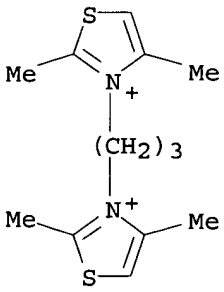
2 I^-

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 54642-17-0 REGISTRY
CN Thiazolium, 3,3'-(1,3-propanediyl)bis[2,4-dimethyl-, diperchlorate (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-3'-Trimethylenebis (2,4-dimethylthiazolium perchlorate
MF C13 H20 N2 S2 . 2 Cl O4
LC STN Files: CA, CAPLUS

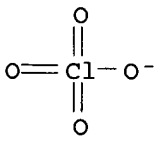
CM 1

CRN 54642-16-9
CMF C13 H20 N2 S2



CM 2

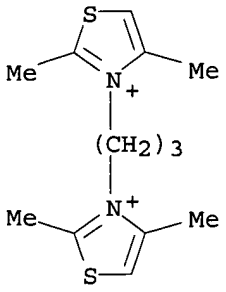
CRN 14797-73-0
CMF Cl O4



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 54642-16-9 REGISTRY
CN Thiazolium, 3,3'-(1,3-propanediyl)bis[2,4-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N2 S2

CI COM



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COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	187.19	190.34

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FILE COVERS 1907 - 5 Feb 2003 VOL 138 ISS 6
FILE LAST UPDATED: 4 Feb 2003 (20030204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l5
L6 9 L5

=> d l6 1-9

L6 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 2001:63952 CAPLUS
DN 134:131521
TI Preparation of neutral prodrugs of bisquaternaryammonium parasiticides
IN Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Bourguignon, Jean-Jacques; Vidal, Valerie; Rubi, Eric
PA Centre National de la Recherche Scientifique (C.N.R.S.), Fr.
SO PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001005742	A1	20010125	WO 2000-FR2122	20000721

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	FR 2796642	A1	20010126	FR 1999-9471	19990721
	FR 2796642	B1	20011019		
	EP 1196371	A1	20020417	EP 2000-958598	20000721
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012601	A	20020521	BR 2000-12601	20000721
PRAI	FR 1999-9471	A	19990721		
	WO 2000-FR2122	W	20000721		

OS MARPAT 134:131521
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1995:786678 CAPLUS
DN 123:313245
TI A kinetic study by NMR of the benzoin condensation catalyzed by thiazolium salts in mild basic conditions: a second order process in both aldehyde and pre-catalyst
AU Lopez-Calahorra, Francisco; Rubires, Raimon
CS Department Quimica Organica, Universitat Barcelona, Barcelona, E-08028, Spain
SO Tetrahedron (1995), 51(35), 9713-28
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English

L6 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1995:36290 CAPLUS
DN 122:9235
TI Use of 3,3'-polymethylene-bridged thiazolium salts plus bases as catalysts of the benzoin condensation and its mechanistic implications: proposal of a new mechanism in aprotic conditions
AU Lopez-Celahorra, Francisco; Castells, Josep; Domingo, Laura; Marti, Josep; Bofill, Josep M.
CS Dep. Quimica Organica, Univ. Barcelona, Barcelona, 08028, Spain
SO Heterocycles (1994), 37(3), 1579-97
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English

L6 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1993:191094 CAPLUS
DN 118:191094
TI New evidence supporting bis(thiazolin-2-ylidene)s as the actual catalytic species in the benzoin condensation
AU Castells, Josep; Domingo, Laura; Lopez-Calahorra, Francisco; Marti, Josep
CS Dep. Quim. Org., Univ. Barcelona, Barcelona, 08028, Spain
SO Tetrahedron Letters (1993), 34(3), 517-20
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English

L6 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1987:84464 CAPLUS
DN 106:84464
TI 3,3'-Tetramethylene-bridged 4-methylthiazolium salt as an organic redox catalyst. The partial reduction of nitrosobenzene with benzaldehyde to azoxybenzene
AU Inoue, Hiroo; Tamura, Shigeo
CS Coll. Eng., Univ. Osaka Prefect., Sakai, 591, Japan
SO Chemistry Express (1986), 1(5), 291-4
CODEN: CHEXEU; ISSN: 0911-9566
DT Journal

LA English

L6 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1986:625923 CAPLUS
DN 105:225923
TI Catalytic function of a 3,3'-tetramethylene-bridged 4-methylthiazolium salt in the reductive cleavage of the sulfur-sulfur bond of disulfides with o-methylbenzaldehyde and bases
AU Inoue, Hiroo; Tamura, Shigeo
CS Dep. Appl. Chem., Univ. Osaka Prefect., Osaka, 591, Japan
SO Journal of the Chemical Society, Chemical Communications (1986), (11), 858-9
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 105:225923

L6 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1985:487566 CAPLUS
DN 103:87566
TI Novel catalytic system consisting of a 3,3'-tetramethylene-bridged 4-methylthiazolium salt leading to the partial reduction of nitrobenzene with benzaldehyde to a nitrone
AU Inoue, Hiroo; Tamura, Shigeo
CS Dep. Appl. Chem., Univ. Osaka Prefect., Osaka, 591, Japan
SO Journal of the Chemical Society, Chemical Communications (1985), (3), 141-2
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 103:87566

L6 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1981:103319 CAPLUS
DN 94:103319
TI A novel base-induced ring expansion of quaternized heterocycles
AU Federsel, Hans Juergen; Bergman, Jan
CS Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SO Tetrahedron Letters (1980), 21(25), 2429-32
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English

L6 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1975:141589 CAPLUS
DN 82:141589
TI Biscyanines with nonconjugated chromophores from 2,4-dimethylthiazole and lepidine derivatives
AU Mushkalo, I. L.; Shedov, I. F.
CS Inst. Org. Khim., Kiev, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1974), (11), 1489-92
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian